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Mixed electronic states of high  $T_c$  cuprates superconductors

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**Abstract**

A model of high  $T_c$  cuprates superconductivity is proposed from the point of view that the electronic state of copper oxides can be described by the fermions constructed with newly defined operators. These operators are composed of  $d$  hole in Cu site and  $p$  hole in O site, and are identified as two types of free fermions. The electronic states are investigated in two cases of nearly non-doped region and the neighborhood of optimally doped region. The interplay between the superconducting and the pseudogap state can be explained by the mixed electronic state which composes of the BCS state and the local antiferromagnetic coupling state. The gap energy and the critical temperature of these states are estimated as a function of the doping quantity, respectively. It is found that Cooper pair formation in high  $T_c$  cuprates superconductors depends on the wave-function overlap of Cu and O holes.

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**Keywords:** High  $T_c$  superconductivity; Pseudogap state; Hubbard model

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**1. Introduction**

High  $T_c$  superconductors (HTS) such as the copper oxides can be generated by electron or hole doping antiferromagnets. It is clear that the doping must play an important role for generating superconductivity. It is also evident that dopant may supply the mobile electrons or holes, that is, carriers in  $\text{CuO}_2$  plane of superconductors. However, in spite of much intensive study about the mechanism of HTS including the early typical theories [1,2], how the doping make an influence on Cooper pair formation still remains an unsolved problem. On the other hand, it has been experimentally reported that there exists above  $T_c$  the so-called “pseudogap” (PG) characterized by a gap-like structure [3]. Since the PG appears in the underdoped region, the interplay between doping and the breakdown of antiferromagnets seems to be indispensable for generating the PG. That is, the doping can induce the two types of electronic states (superconductivity and PG). It is so hopeful to reveal not only the mechanism of Cooper pair formation but also the relation between superconductivity and pseudogap state. Here, a model of high  $T_c$  cuprates superconductivity is presented, based on the  $d$ - $p$  model emphasizing that the electronic state of copper oxides can be described by the fermions constructed with newly defined operators.

**2. Formulation**

It will be assumed that the Hamiltonian is given by an extended Hubbard model for a single layer of square planar

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coordinated Cu and O atoms:

$$H = \sum_i \varepsilon_d d_{i\sigma}^+ d_{i\sigma} + \sum_j \varepsilon_p p_{j\sigma}^+ p_{j\sigma} + \sum_i \sum_{j \in \{i\}} (\varepsilon_{ij} d_{i\sigma}^+ p_{j\sigma} + \text{H.c.}) + U \sum_i d_{i\uparrow}^+ d_{i\uparrow} d_{i\downarrow}^+ d_{i\downarrow} + \sum_{ij\sigma\sigma'} V_{\sigma\sigma'} d_{i\sigma}^+ d_{i\sigma} p_{j\sigma'}^+ p_{j\sigma'}, \quad (1)$$

where the operator  $d_{i\sigma}^+$  creates Cu ( $3d_{x^2-y^2}$ ) holes at site  $i$ ,  $p_{j\sigma}^+$  creates O ( $2p_x, 2p_y$ ) holes at site  $j$ ,  $\varepsilon_d = 0$ , and  $\varepsilon_{ij}$  is the nearest-neighbor hopping integral.  $U$  is the on-site Coulomb repulsion at a Cu site, and  $V_{\sigma\sigma'}$  is the interaction between neighboring Cu and O sites. In Eq. (1), the vacuum is defined as filled Cu  $d^{10}$  and O  $p^6$  states. The peculiarity in this study is to consider two cases of nearly non-doped region (PG region) and the neighborhood of optimally doped region (superconductive region), separately. First let us consider the case of the nearly non-doped region. Here the operator  $d_{i\sigma}^+$ ,  $p_{j\sigma}^+$  are reconstructed with newly defined fermion operators as shown in

$$b_{i\sigma}^+ = \alpha d_{i\sigma}^+ + \beta \tilde{p}_{i\sigma}^+, \quad c_{i\sigma}^+ = \beta d_{i\sigma}^+ - \alpha \tilde{p}_{i\sigma}^+, \quad \tilde{p}_{i\sigma}^+ = \frac{1}{2} \sum_{j \in \{i\}} \frac{\varepsilon_{ij}}{|\varepsilon_{ij}|} p_{j\sigma}^+, \quad \alpha^2 + \beta^2 = 1, \quad (2)$$

where  $b_{i\sigma}^+$ ,  $c_{i\sigma}^+$  are the mixing operators of Cu and O holes and satisfy anti-commutation relations, respectively. The operator  $\tilde{p}_{i\sigma}^+$  is so defined as Zhang and Rice's treatment of  $d$ - $p$  model [4], and  $\varepsilon_{ij}$  is given by  $\varepsilon_{ij} = -\varepsilon < 0$  ( $j = 1, 2$ ),  $\varepsilon > 0$  ( $j = 3, 4$ ). If  $\sum_{j\sigma} p_{j\sigma}^+ p_{j\sigma} \approx 2 \sum_{i\sigma} \tilde{p}_{i\sigma}^+ \tilde{p}_{i\sigma}$ ,  $\alpha\beta\varepsilon_p = \varepsilon(\beta^2 - \alpha^2)$  are satisfied, the Hamiltonian (1) is transformed into

$$H = \frac{2\varepsilon_p}{\beta^2 - \alpha^2} \sum_{i\sigma} (\beta^2 b_{i\sigma}^+ b_{i\sigma} - \alpha^2 c_{i\sigma}^+ c_{i\sigma}) + U \sum_i (\alpha^4 b_{i\uparrow}^+ b_{i\uparrow} b_{i\downarrow}^+ b_{i\downarrow} + \alpha^2 \beta^2 b_{i\uparrow}^+ b_{i\uparrow} c_{i\downarrow}^+ c_{i\downarrow} + \alpha^2 \beta^2 c_{i\uparrow}^+ c_{i\uparrow} b_{i\downarrow}^+ b_{i\downarrow} + \beta^4 c_{i\uparrow}^+ c_{i\uparrow} c_{i\downarrow}^+ c_{i\downarrow} + \dots) + \sum_{i\sigma\sigma'} V_{\sigma\sigma'} (\alpha^2 \beta^2 b_{i\sigma}^+ b_{i\sigma} b_{i\sigma'}^+ b_{i\sigma'} + \alpha^4 b_{i\sigma}^+ b_{i\sigma} c_{i\sigma'}^+ c_{i\sigma'} + \beta^4 c_{i\sigma}^+ c_{i\sigma} b_{i\sigma'}^+ b_{i\sigma'} + \alpha^2 \beta^2 c_{i\sigma}^+ c_{i\sigma} c_{i\sigma'}^+ c_{i\sigma'} + \dots). \quad (3)$$

Here the Hamiltonian consists of the atomic energy of composite fermions, Coulomb repulsion and the interaction between them. The many experimental facts indicate that the copper oxides show antiferromagnets in the non-doped region [5,6]. It is so well known that the ground state of the antiferromagnets corresponds to the so-called Mott insulator. Using the composite operators defined here, the non-doped wave function is represented as

$$|\Psi_{MI}\rangle = \prod_{i \in A}^{N/2} (\alpha b_{i\uparrow}^+ + \beta c_{i\uparrow}^+) \prod_{i' \in B}^{N/2} (\alpha b_{i'\downarrow}^+ + \beta c_{i'\downarrow}^+) |0\rangle, \quad (4)$$

where  $A$  or  $B$  shows the sub-space of antiferromagnetic lattice and  $N$  is number of Cu sites in a single layer. There exists no  $p$ -hole in half-filling Mott insulator. In Hamiltonian (3), if  $V_{\sigma\sigma'}$  is negative, the attractive interaction terms will play an important role for determining the ground state. Doping holes can be expected to occupy the quantum state corresponding to this situation. For the relation  $\alpha < \beta$  which allows the reliable value of  $\varepsilon_p, \varepsilon$ , the term  $b_{i\sigma}^+ b_{i\sigma} c_{i\sigma'}^+ c_{i\sigma'} (c_{i\sigma}^+ c_{i\sigma} b_{i\sigma'}^+ b_{i\sigma'})$  can be the most attractive interaction. This suggests that  $b$ - $c$  or  $c$ - $b$  pair will mainly contribute to determine the ground state. Thus, under the attractive interaction of  $2\alpha^2\beta^2U + 2(\alpha^4 + \beta^4)V < 0$  including antiferro-coupling ( $V = V_{\uparrow\downarrow} < 0$ ) and equivalency of sites, the wave function is assumed to be

$$|\Psi_A\rangle = \prod_i (s + t b_{i\uparrow}^+ c_{i\downarrow}^+) (s + t c_{i\uparrow}^+ b_{i\downarrow}^+) |\Psi_{MI}\rangle, \quad s^2 + t^2 = 1, \quad (5)$$

where the coefficient  $t$  indicates the probability of local-antiferro pair state. The ground-state energy is then given by

$$E = \langle \Psi_A | H | \Psi_A \rangle = 4s^2 t^2 [\varepsilon_p + 0.5U(1 - 2\alpha^2\beta^2) + V]. \quad (6)$$

Approximating that the doping can only supply the  $p$ -holes, the value of  $st$  is determined by using the relation  $\langle \Psi_A | \sum_{i\sigma} 2\tilde{p}_{i\sigma}^+ \tilde{p}_{i\sigma} | \Psi_A \rangle = 4s^2 t^2 = \delta$  (the doping ratio relative to half-filling). In (6) the term  $|0.5U(1 - 2\alpha^2\beta^2) + V|$  is roughly estimated to be the excitation energy from local-antiferro pair state per one hole. Identifying the excitation energy as the so-called pseudogap, this state can be interpreted as the pseudogap state because it is regarded as the electronic state containing the local antiferro-coupling. Second consider the case of the neighborhood of optimally doped region. Since the band picture is appropriate in this case, Hamiltonian (1) is rewritten as in momentum space

$$H = \sum_{\mathbf{k}\sigma} \varepsilon_d d_{\mathbf{k}\sigma}^+ d_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \varepsilon_p p_{\mathbf{k}\sigma}^+ p_{\mathbf{k}\sigma} + \sum_{\mathbf{k}\sigma} \frac{1}{\sqrt{2}} \varepsilon s(\mathbf{k}) (-i d_{\mathbf{k}\sigma}^+ p_{\mathbf{k}\sigma} + i p_{\mathbf{k}\sigma}^+ d_{\mathbf{k}\sigma}) + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} d_{\mathbf{k}\uparrow}^+ d_{\mathbf{k}'\uparrow} d_{\mathbf{q}-\mathbf{k}\downarrow}^+ d_{\mathbf{q}-\mathbf{k}'\downarrow} + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} V_{\sigma\sigma'} \theta(\mathbf{k}-\mathbf{k}') d_{\mathbf{k}\sigma}^+ d_{\mathbf{k}'\sigma} p_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'}^+ p_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'}, \quad (7)$$

where  $s(\mathbf{k}) = (s \sin k_x + s \sin k_y)$ ,  $\theta(\mathbf{k}) = (c \cos k_x + c \cos k_y)$ , and the Cu-O distance is used as the length unit. Again, the operators  $d_{\mathbf{k}\sigma}^+$ ,  $p_{\mathbf{k}\sigma}^+$  are reconstructed with newly defined fermion operators as shown in

$$b_{\mathbf{k}\sigma}^+ = \alpha_k d_{\mathbf{k}\sigma}^+ + i\beta_k p_{\mathbf{k}\sigma}^+, \quad c_{\mathbf{k}\sigma}^+ = \beta_k d_{\mathbf{k}\sigma}^+ - i\alpha_k p_{\mathbf{k}\sigma}^+, \quad \alpha_k^2 + \beta_k^2 = 1. \quad (8)$$

Under the condition of  $\sqrt{2}\alpha_k\beta_k\varepsilon_p = \varepsilon s(\mathbf{k})(\beta_k^2 - \alpha_k^2)$ , the Hamiltonian (7) is transformed into

$$H = \sum_{\mathbf{k}\sigma} \frac{\varepsilon_p}{\beta_k^2 - \alpha_k^2} (\beta_k^2 b_{\mathbf{k}\sigma}^+ b_{\mathbf{k}\sigma} - \alpha_k^2 c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}\sigma}) + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} (\alpha_k \alpha_{\mathbf{k}'} \alpha_{\mathbf{q}-\mathbf{k}} \alpha_{\mathbf{q}-\mathbf{k}'} b_{\mathbf{k}\uparrow}^+ b_{\mathbf{k}'\uparrow}^+ b_{\mathbf{q}-\mathbf{k}\downarrow} b_{\mathbf{q}-\mathbf{k}'\downarrow} + \alpha_k \alpha_{\mathbf{k}'} \beta_{\mathbf{q}-\mathbf{k}} \beta_{\mathbf{q}-\mathbf{k}'} b_{\mathbf{k}\uparrow}^+ b_{\mathbf{k}'\uparrow}^+ c_{\mathbf{q}-\mathbf{k}\downarrow}^+ c_{\mathbf{q}-\mathbf{k}'\downarrow}^+ + \alpha_{\mathbf{q}-\mathbf{k}} \alpha_{\mathbf{q}-\mathbf{k}'} \beta_k \beta_{\mathbf{k}'} c_{\mathbf{k}\uparrow}^+ c_{\mathbf{k}'\uparrow}^+ \beta_{\mathbf{q}-\mathbf{k}\downarrow} \beta_{\mathbf{q}-\mathbf{k}'\downarrow} + \beta_k \beta_{\mathbf{k}'} \beta_{\mathbf{q}-\mathbf{k}} \beta_{\mathbf{q}-\mathbf{k}'} c_{\mathbf{k}\uparrow}^+ c_{\mathbf{k}'\uparrow}^+ c_{\mathbf{q}-\mathbf{k}\downarrow} c_{\mathbf{q}-\mathbf{k}'\downarrow} + \dots) + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} V_{\sigma\sigma'} \theta(\mathbf{k}-\mathbf{k}') (\alpha_k \alpha_{\mathbf{k}'} \beta_{\mathbf{k}-\mathbf{k}'} \beta_{\mathbf{k}-\mathbf{k}'} b_{\mathbf{k}\sigma}^+ b_{\mathbf{k}'\sigma}^+ b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'}^+ b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'} + \alpha_k \alpha_{\mathbf{k}'} \alpha_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'} b_{\mathbf{k}\sigma}^+ b_{\mathbf{k}'\sigma}^+ c_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'}^+ c_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'} + \beta_{\mathbf{k}} \beta_{\mathbf{k}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma}^+ b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'}^+ b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'} + \beta_{\mathbf{k}} \beta_{\mathbf{k}'} \alpha_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'} c_{\mathbf{k}\sigma}^+ c_{\mathbf{k}'\sigma}^+ c_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'}^+ c_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'} + \dots). \quad (9)$$

Note that in (9)  $b_{\mathbf{k}\sigma}^+$  or  $c_{\mathbf{k}\sigma}^+$  fermion has the possibility of creating Cooper pairs, but for  $\alpha_k < \beta_k$  the interaction between  $c_{\mathbf{k}\sigma}^+$  fermions will probably be repulsive. Assuming that  $b_{\mathbf{k}\sigma}^+$  fermions contribute to the Cooper formation, (9) is approximated as

$$H = \sum_{\mathbf{k}\sigma} \frac{\varepsilon_p}{\beta_k^2 - \alpha_k^2} \beta_k^2 b_{\mathbf{k}\sigma}^+ b_{\mathbf{k}\sigma} + \frac{U}{N} \sum_{\mathbf{k}\mathbf{k}'\mathbf{q}} \alpha_k \alpha_{\mathbf{k}'} \alpha_{\mathbf{q}-\mathbf{k}} \alpha_{\mathbf{q}-\mathbf{k}'} b_{\mathbf{k}\uparrow}^+ b_{\mathbf{k}'\uparrow}^+ b_{\mathbf{q}-\mathbf{k}\downarrow} b_{\mathbf{q}-\mathbf{k}'\downarrow} + \frac{1}{N} \sum_{\mathbf{k}\mathbf{k}'\sigma\sigma'} V_{\sigma\sigma'} \theta(\mathbf{k}-\mathbf{k}') \alpha_k \alpha_{\mathbf{k}'} \beta_{\mathbf{k}-\mathbf{k}'} \beta_{\mathbf{k}-\mathbf{k}'} b_{\mathbf{k}\sigma}^+ b_{\mathbf{k}'\sigma}^+ b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'}^+ b_{\mathbf{k}-\mathbf{k}'+\mathbf{k}'\sigma'} + \dots \quad (10)$$

Considering that the ground state is superconductive in the neighborhood of optimally doped region, the BCS-like wave function is given by

$$|\Psi_s\rangle = \prod_{\mathbf{k}} (u_{\mathbf{k}} + v_{\mathbf{k}} b_{\mathbf{k}\uparrow}^+ b_{\mathbf{k}\downarrow}^+) |0\rangle, \quad u_{\mathbf{k}}^2 + v_{\mathbf{k}}^2 = 1. \quad (11)$$

The ground-state energy is

$$F = \langle \Psi_s | H | \Psi_s \rangle = 2 \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} v_{\mathbf{k}}^2 + \sum_{\mathbf{k}\mathbf{k}'} [U \alpha_{\mathbf{k}}^2 \alpha_{\mathbf{k}'}^2 + V \alpha_{\mathbf{k}} \alpha_{\mathbf{k}'} \beta_{\mathbf{k}} \beta_{\mathbf{k}'} \theta(\mathbf{k}-\mathbf{k}')] u_{\mathbf{k}} v_{\mathbf{k}'} v_{\mathbf{k}'}, \quad (12)$$

where  $U \alpha_{\mathbf{k}}^2 \alpha_{\mathbf{k}'}^2 + V \alpha_{\mathbf{k}} \alpha_{\mathbf{k}'} \beta_{\mathbf{k}} \beta_{\mathbf{k}'} \theta(\mathbf{k}-\mathbf{k}')$  is assumed to be attractive. The relation  $\varepsilon_{\mathbf{k}} = 0.5(\varepsilon_p + \sqrt{2\varepsilon^2 s^2(\mathbf{k}) + \varepsilon_p^2}) - \mu$  is defined, measuring the energy relative to the Fermi level  $\mu$ . By minimizing  $F$  with respect to  $u_{\mathbf{k}}, v_{\mathbf{k}}$ , the following gap equation is given by

$$\Delta_{\mathbf{k}} = -\frac{1}{2} \sum_{\mathbf{k}'} \frac{\Delta_{\mathbf{k}'}}{E_{\mathbf{k}'}} V_{\mathbf{k}\mathbf{k}'}, \quad E_{\mathbf{k}} = \sqrt{\Delta_{\mathbf{k}}^2 + \varepsilon_{\mathbf{k}}^2}, \quad V_{\mathbf{k}\mathbf{k}'} = U \alpha_{\mathbf{k}}^2 \alpha_{\mathbf{k}'}^2 + V \alpha_{\mathbf{k}} \alpha_{\mathbf{k}'} \beta_{\mathbf{k}} \beta_{\mathbf{k}'} \theta(\mathbf{k}-\mathbf{k}'). \quad (13)$$

For simplicity neglecting the Coulomb repulsion and replacing the sum in (13) by an integral, the solution which is even in  $\mathbf{k}$  is given by  $\Delta_{\mathbf{k}} = \Delta_0 \alpha_{\mathbf{k}} \beta_{\mathbf{k}} (\cos k_x \pm \cos k_y)$ . Considering  $\Delta_{\mathbf{k}} \propto \cos k_x - \cos k_y$  which is the experimental fact about the anisotropic superconductive gap [7],  $\Delta_0$  is determined by the following relation.

$$-\frac{8\pi^2}{V} = \int \frac{\alpha_{\mathbf{k}}^2 \beta_{\mathbf{k}}^2 (\cos k_x - \cos k_y) \cos k_x}{\sqrt{\Delta_0^2 \alpha_{\mathbf{k}}^2 \beta_{\mathbf{k}}^2 (\cos k_x - \cos k_y)^2 + \varepsilon_{\mathbf{k}}^2}} d\mathbf{k}. \quad (14)$$

Using the value of  $\Delta_0$  calculated from (14), the ground-state energy  $F$  is obtained.

### 3. Mixed electronic states

Since the formulation in Section 2 is only constructed in two special cases of nearly non-doped and the neighborhood of optimally doped regions, the results cannot be exactly applied to the case of the intermediate doped region. In order to evaluate the intermediate region, it is indispensable to investigate how the ground-state energy depends on the doping-ratio  $\delta$  in these two regions. First consider the doping effect in the case of the nearly non-doped region. Increasing of the doping quantity will generally change the possibility of  $d$ - $p$  transition. As a result,  $\alpha$  and  $\beta$  will also change with the value of  $\delta$ . It is assumed here that the effective hopping parameter is  $\varepsilon \rightarrow \varepsilon_0(1-\delta)$  and anti-ferromagnetic exchange interaction is  $V \rightarrow \varepsilon^2 V_0$ . Thus, the ground-state energy  $E(\delta)$  and the pseudogap  $\Delta_{\text{PG}}$  are approximately obtained as a function of  $\delta$ :

$$E(\delta) = \delta \left[ \varepsilon_p + \frac{[\varepsilon_0^2(1-\delta)^2 + 0.5\varepsilon_p^2]U}{4\varepsilon_0^2(1-\delta)^2 + \varepsilon_p^2} + \varepsilon_0^2(1-\delta)^2 V_0 \right], \quad \Delta_{\text{PG}} = \left| \frac{[\varepsilon_0^2(1-\delta)^2 + 0.5\varepsilon_p^2]U}{4\varepsilon_0^2(1-\delta)^2 + \varepsilon_p^2} + \varepsilon_0^2(1-\delta)^2 V_0 \right|. \quad (15)$$

Next consider the case of the neighborhood of optimally doped regions. Let us try the estimation of  $\Delta_0$  in (14) considering the neighborhood of  $k_x = k, k_y = 0.5\pi$  on the Fermi surface. In this approximation, (14) is transformed into

$$-\frac{8\pi^2}{V} = \int_0^{\varepsilon_0} \frac{2\pi C^2}{\sqrt{C^2 \Delta_0^2 + \xi^2}} \frac{dk}{d\delta} \frac{d\delta}{d\xi} d\xi, \quad C = \frac{\varepsilon(\sin k + 1) \cos k}{\sqrt{2}\varepsilon_p}, \quad (16)$$

where  $E_0$  is the energy width contributing to the Cooper formation. Identifying  $d\delta/d\xi$  as the density of states  $N_F$  at Fermi level, the superconductive gap is obtained by solving (16) as follow as

$$\Delta_m = \alpha_k \beta_k \Delta_0 = \frac{E_0}{\sinh[-D/N_F V]}, \quad D = \frac{8\pi\epsilon_p^2}{\epsilon^2 \cos^2 k (1 + \sin k)^2} \cdot \frac{d\delta}{dk}. \quad (17)$$

The relation  $k \approx \pi\delta/6$  on the Fermi surface is approximately estimated from the two-dimensional band structure. Using the relations of  $V = \epsilon^2 V_0$ ,  $\epsilon = \epsilon_0 (1 - \delta)$ ,  $N_F = n_0 \delta$ ,  $\Delta_m$  becomes a function of  $\delta$  and its value initially increases with increasing of  $\delta$ , and passing through the maximum point, begins to decrease. The maximum value of  $\Delta_m$  is corresponding to the optimally doped point, and is estimated to  $\delta \approx 0.2$  by rough calculation. The ground-state energy is also obtained as a function of  $\delta$ .

$$F(\delta) = \delta \left[ \epsilon_p + \frac{\epsilon_0^2 (1 - \delta)^2}{\epsilon_p} \int_0^{E_F} S(\xi) d\xi \right] - \frac{1}{2} n_0 \delta \cos^2(\pi\delta/6) \Delta_m^2(\delta), \quad (18)$$

where the energy relative to Cu3d level is measured and  $S(\xi)$  is a function indicating the normal state below Fermi level. Let us compare the ground-state energy  $E(\delta)$  in (15) with  $F(\delta)$  in (18). If  $V = 0$ ,  $E(\delta)$  is estimated to be larger than  $F(\delta)$ . Thus, the band-like state seems to be more stable than the pseudogap state. However, in the presence of  $V < 0$  the situation will become more different. Since the experimental facts reveal that the nearly non-doped region indicates the pseudogap state, there can be the mixed state in the intermediate region. This region is determined by the condition of  $\partial E(\delta)/\partial \delta|_{\delta=\delta_A} = \partial F(\delta)/\partial \delta|_{\delta=\delta_S}$  which means the same chemical potential in two states. It is assumed that superconductivity appears in the pseudogap state at  $\delta_A$ , and the mixed state becomes a single superconductor at  $\delta_S$ . This assumption is consistent with the recent research in which the pseudogap state competes with the superconductivity [8]. In this doped region the wave function will be approximately represented as the mixing of localized antiferro-coupling and superconductive state:

$$|\Psi_I(\delta)\rangle = \sqrt{\frac{\delta_S - \delta}{\delta_S - \delta_A}} |\Psi_A(\delta)\rangle + \sqrt{\frac{\delta - \delta_A}{\delta_S - \delta_A}} |\Psi_S(\delta)\rangle. \quad (19)$$

Now let us estimate the doping dependency of the model. As shown in (15), the PG gap decreases with increasing of  $\delta$  in the region of  $0 < \delta < \delta_A$ .  $T^*$  (PG critical temperature) will also show a similar tendency. For  $\delta_A < \delta < \delta_S$ , the doping dependency will show the same tendency. On the other hand, the superconductive state appears at  $\delta = \delta_A$ , and in the region of  $\delta_A < \delta < \delta_S$ , its ratio increases more with increasing of  $\delta$ . The superconductive gap  $\Delta_m$  is increasing from  $\Delta_m(\delta_A)$  and becomes  $\Delta_m(\delta_S)$  at  $\delta = \delta_S$ . However,  $T_c$  will not be directly determined by the gap  $\Delta_m$  since the coherency in the superconductor becomes weak due to the mixing states.  $T_c$  in the region of  $\delta_A < \delta < \delta_S$  is assumed to be determined by the effective maximum gap defined as  $\Delta_{eff} = \sqrt{(\delta - \delta_A)/(\delta_S - \delta_A)} \Delta_m(\delta)$ . Thus,  $T_c = 0$  at  $\delta = \delta_A$  and increases with  $\delta$ . Though  $\delta_S$  seems to be almost the optimally doped point  $\delta_P$ , if  $\delta_S < \delta_P$ ,  $T_c$  shows the maximum value at  $\delta = \delta_P$ . In the over-doped region, since  $\Delta_m$  decreases with  $\delta$  and there is no mixing state in this region,  $T_c$  will also decrease with the decrease of  $\Delta_m$ . I feel that these results are consistent with the experimental facts. However, in order to confirm them, the numerical evaluation will be needed in detail.

#### 4. Conclusions

The electronic state of high  $T_c$  cuprates superconductors is investigated by using the model which can be described by the fermions constructed with newly defined operators. The interplay between the superconducting and the pseudogap state can be explained by the mixed electronic state which composes of the BCS state and the local antiferromagnetic coupling state. The gap energy and the critical temperature of these states are estimated as a function of the doping quantity, and the results are consistent with the experimental facts. The much interest is that Cooper pair formation depends on the wave-function overlap of Cu and O holes. This may provide an important hint enhancing  $T_c$  of various cuprates superconductors.

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